Fractals to model hierarchical materials and structures

FRACTALS TO MODEL HIERARCHICAL MATERIALS AND STRUCTURES

Alberto Carpinteri*, Nicola Pugno, Alberto Sapora

Department of Structural Engineering and Geotechnics, Politecnico di Torino,
Corso Duca degli Abruzzi 24, 10129 Torino, Italy.

*alberto.carpinteri@polito.it

Keywords: hierarchical materials, structures, fractals, strain energy, rigidity

SUMMARY. Many materials exhibit microstructure on more than one length scale. In the present paper we face the problem of hierarchical materials and structures by means of a fractal approach. We firstly propose a mathematical model to design nano-inspired hierarchical materials. Simple formulas describing the dependence of strength, toughness and stiffness are derived. The problem of hierarchical beam-framed structures is then considered. Basic energy considerations seem to suggest peculiar scaling laws for the geometric and mechanical features of the structure.

1 INTRODUCTION

The hierarchical order of a material (or a structure) can be viewed as the number $n=N$ of scale levels with recognized structure. For $n=0$ the material is viewed as homogeneous.

Biological materials exhibit several levels of hierarchy, from the micro- to the macro-scale. For instance, sea shells have 2 or 3 orders of lamellar structures, as well as bone, similarly to dentin, has 7 orders of hierarchy [Currey, 1977,1984]. These materials are composed by hard and strong mineral structures embedded in a soft and tough protein matrix. In bone and dentin, the mineral platelets are ~3nm thick, whereas in shells their thickness is of ~300nm, with very high slenderness. With this hard/soft hierarchical texture, Nature seems to suggest us the key for optimizing materials with respect to both strength and toughness, without losing stiffness. Even if hierarchical materials are recognized to possess a fractal-like topology [Lakes, 1993], only few engineering models explicitly considering their complex structure are present in the literature (see [Gao, 2006] and related references). In the next section alternative and concise mathematical models will be presented, based on our previous experience on fractal geometry [Carpinteri and Pugno, 2005,2007].

The attention is then turned to the mechanical behaviour of hierarchical beam-framed structures. The structural response of a von Koch cantilever beam, an archetype of self-similar structures, is analyzed under different loading conditions in the small-deformation regime. Simple recursive formulas on the strain energy are derived, which show us the rate at which structural features should scale in order to prevent compliance divergence.

2 HIERARCHICAL MATERIALS

Let us consider a tensile test on a hierarchically fibre-reinforced bar. Its cross-section, composed by hard inclusions embedded in a soft matrix, is schematized in Figure 1.

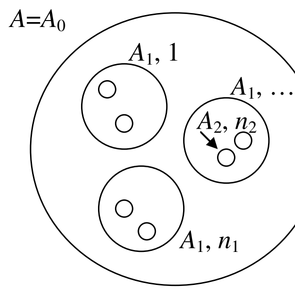

Figure 1. The cross-section of a hierarchical bar.

Each inclusion at the level $k-1$ contains n_k smaller ones, each of them with cross-sectional area A_k. Thus, the total number of inclusions at the level *k* is $N_k = \prod_{j=1}^{k} n_j$. The smallest units, at the level *N*, are considered scale-invariant. Finally, let us denote with $\varphi_k = \frac{n_{k+1} A_{k+1}}{A_k}$ the cross-sectional fraction of the inclusions at the level *k*+1 inside the inclusion at the level *k*.

Natural optimization suggests self-similar structures [Brown and West, 2000], for which $n_k = n$ and $\varphi_k = \varphi$, and thus *k*-independent numbers and fractions. Accordingly, $N_k = n^k$.

The *equilibrium equation* is:

$$F \equiv A\sigma_C = F_h + F_s = N_k A_k \sigma_{hk} + (A - N_k A_k)\sigma_{sk} = N_N A_N \sigma_{hN} + (A - N_N A_N)\sigma_{sN}, \ \forall k$$

where *F* is the critical applied force and F_h, F_s are the forces carried by the hard and soft phases respectively; $A \equiv A_0$ is the cross-section area of the bar, σ_C is its strength; $\sigma_{hN} \equiv \sigma_h$, $\sigma_{sk} \equiv \sigma_s$ ($\forall k$), σ_h, σ_s, are the material strengths of the hard and soft phases, respectively; the subscript *k* simply refers to the quantities at the level *k*.

Since the inclusions present a fractal distribution [Carpinteri and Pugno, 2005], we expect $F_h \propto R^D$ where $R = \sqrt{A}$ is a characteristic size and *D* is a constant, the so-called "fractal exponent". The constant of proportionality can be deduced noting that $F_h(A = A_N) = A_N \sigma_{hN}$, and thus $F_h = \sigma_{hN} R_N^{2-D} R^D$. Accordingly, from $F_h = \sigma_{hN} R_N^{2-D} R^D = \sigma_{hN} n^N R_N^2$, we derive:

$$N = D\frac{\ln R/R_N}{\ln n}, \tag{1}$$

which defines the number of hierarchical levels that we need to design an object of characteristic size *R*. Eqn.(1) shows that only few hierarchical levels are required for spanning several orders of magnitude in size.

The scaling exponent *D* can be determined noting that $A - N_N A_N = A(1-\phi)$, where $\phi = \varphi^N$ represents the macroscopic (at level 0) cross-sectional fraction of the hard inclusions. Thus, we derive $R/R_N = (n/\varphi)^{N/2}$. Introducing this result into eqn.(1) provides the fractal exponent, as a function of well-defined physical quantities:

$$D = \frac{2\ln n}{\ln n - \ln \varphi}. \tag{2}$$

Noting that $n > 1$ and $\varphi < 1$, we deduce 0<*D*<2. *D* represents the fractal dimension of the inclusions, i.e., of a lacunar two-dimensional domain in which the soft matrix is considered as empty [Carpinteri 1994, 1994b]. For example, the dimension of the well-known Sierpinski carpet (Figure 2), is *D*=1.89.

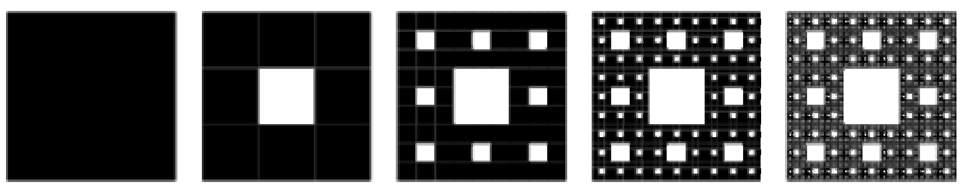

Figure 2. The Sierpinski carpet (*D*=1.89) at different levels of observation; it corresponds to a deterministic hierarchical bar in which the empty space is the soft matrix, and the complementary zones are the hard inclusions.

By substituting

$$\phi = \varphi^N = (R/R_N)^{D-2} \tag{3}$$

into eqn.(1), it yields:

$$\sigma_C = \sigma_h \varphi^N + \sigma_s\left(1-\varphi^N\right) = \sigma_h (R/R_N)^{D-2} + \sigma_s\left(1-(R/R_N)^{D-2}\right). \tag{4}$$

Eqn.(4) represents a scaling law for strength; taking into account that usually $\sigma_h >> \sigma_s$, eqn.(4) predicts that strength decreases as the size increases (Figure 3).

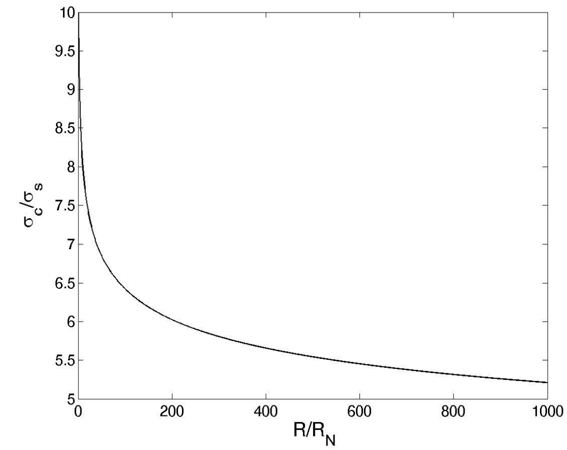

Figure 3. Strength σ_C scaling law (dimensionless quantities) for σ_h/σ_s=10 and D=1.89.

On the other hand, the *energy balance* and the *compatibility equation* provide the scaling equations of the unit fracture energy G_C and of the Young's modulus E of the bar. In formulae:

$$G_C = G_h\varphi^N + G_s\left(1-\varphi^N\right) = G_h\left(R/R_N\right)^{D-2} + G_s\left(1-\left(R/R_N\right)^{D-2}\right), \tag{5}$$

$$E = E_h\varphi^N + E_s\left(1-\varphi^N\right) = E_h\left(R/R_N\right)^{D-2} + E_s\left(1-\left(R/R_N\right)^{D-2}\right), \tag{6}$$

where G_h, G_s and E_h, E_s are the unit fracture energies and Young's moduli of the bar, hard and soft phases, respectively. Since usually $G_h << G_s$ and $E_h >> E_s$, eqns. (5-6) state that, as the size increases, the fracture energy increases (Figure 4) and the stiffness decreases.
The scaling laws predicted by eqns.(4-6) show two asymptotic behaviours, for macro and micro size-scales; note that they all present the same self-consistent form:

$$X \equiv X_0 = X_h\varphi^N + X_s\left(1-\varphi^N\right), \tag{7}$$

where X is the generic property.
The model could be easily extended to a three-dimensional architecture.
Furthermore, for quasi-fractal hierarchy, described by $n(R)$ and $\varphi(R)$ weakly varying with the size R, function $D(R)$ should be considered in eqns.(4-6), as deducible from eqn.(2).

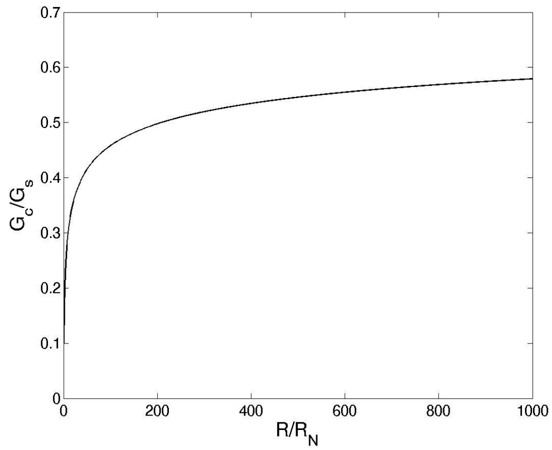

Figure 4. Fracture energy G_C scaling law (dimensionless quantities) for G_s/G_h=10 and D=1.89.

3 HIERARCHICAL BEAM-FRAMED STRUCTURES

In order to understand the behaviour of hierarchical beam-framed structures, we will refer to the classical Von Koch curve, whose features are briefly described in the following section.

3.1 TRIADIC VON KOCH BEAM

Let us recall the properties of the triadic von Koch curve [Feder, 1988]. The construction of the von Koch curve starts with a line segment of length l. At the first generation the set consists of the four segments of length $l/3$, obtained removing the middle third of the generator and replacing it by the other two sides of the equilateral triangle based on the removed segment. This procedure is iterated ad infinitum: at each stage the middle third of each interval is replaced by the other two sides of an equilateral triangle. At the n-th step, the number of segments is 4^n with length $l_n=1/3^n$; thus the total length L_n is $(4/3)^n l$. As n tends to infinity the sequence of the polygonal curves obtained iteration by iteration approaches a limiting curve, called the von Koch curve. This is clearly a self-similar set: it is made of four "quarters", each similar to the whole, but scaled by a factor 1/3. Its fractal dimension can be determined, by exploiting the property of self-similarity, as the ratio of the logarithm of the number of copies to the logarithm of the scaling factor. Thus, the fractal dimension of the triadic von Koch curve is $D=\ln 4/\ln 3$.

3.2 VON KOCH CANTILEVER BEAM SUBJECTED TO A COUPLE AT THE FREE END

Let us now consider a rectilinear cantilever beam subjected to a couple m at the free end. The beam is placed in a Cartesian (x,y) coordinate system in such a way that the left clamped end of the beam is at the origin and the right end, where the couple m is applied, at the point with coordinates $(l,0)$ (Figure 5).

The moment M diagram is constant and equal to m, while the shear stress T is identically equal to zero. Focussing our attention to a small deformation regime and assuming a linear elastic isotropic response, the strain energy Φ_0 related to such a structure could be easily evaluated as [Carpinteri 1992]:

$$\Phi_0 = \frac{1}{2}\int_S \frac{M^2}{EI}dx = \frac{1}{2}\int_0^l \frac{m^2}{EI}dx = \frac{m^2 l}{2EI}, \tag{8}$$

where S is the structure, E is the Young's modulus and I is the moment of inertia.
By applying Castigliano's Theorem, it is then possible to calculate the displacements at the free end; for example, as regards the rotation $\varphi_{0,}$ it is easy to obtain:

$$\varphi_0(x = l) = \frac{\partial \Phi_0}{\partial m} = \frac{ml}{EI}. \tag{9}$$

The vertical displacement $v_0(x=l)$ could then be obtained from eqn.(9), by means of a simple integration procedure.
On the other hand, if the beam has a self-similar structure, much more can be said about the strain energy and new physical considerations rise up. Henceforth, we will refer to the product $k=EI$ as the beam rigidity. Moreover, the rotation $\varphi(x = l)$ at the free end (and the displacement $v(x=l)$) will be denoted merely by φ (and v).
As already said, at the generation step the von Koch curve can be seen as the disjoint union of four identical parts, each of which reduced by a factor 3 from the original. In the case of the free-end couple, each part is subjected to the same moment m (Figure 5); hence, it is not difficult to obtain a recursive formula for the strain energy at each stage:

1. $\Phi_1 = 4\left(\frac{1}{2}\int_0^{l/3} \frac{M^2}{EI}dx\right) = \frac{4m^2 l}{6EI} = \frac{4}{3}\Phi_0$

2. $\Phi_2 = 16\left(\frac{1}{2}\int_0^{l/9} \frac{M^2}{EI}dx\right) = \frac{16m^2 l}{18EI} = \left(\frac{4}{3}\right)^2 \Phi_0$

$$\vdots$$

n. $$\Phi_n = 4^n\left(\frac{1}{2}\int_0^{l/3^n} \frac{M^2}{EI}dx\right) = \left(\frac{4}{3}\right)^n \Phi_0, \tag{10}$$

where Φ_0 is provided by eqn.(8). Eqn.(10) shows that, if the rigidity $k=EI$ (implicitly embedded in the function Φ_0) keeps constant, the strain energy Φ_n increases at each iteration step of the von Koch curve. More in detail, it is evident that the strain energy Φ_n scales exactly as the length L_n does. For n tending to infinity, the structural stiffness tends to zero and the beam becomes infinitely compliant. As deducible from eqn.(9):

$$\lim_{n\to\infty} \varphi_n = \lim_{n\to\infty}\left(\frac{4}{3}\right)^n \varphi_0 = \infty . \tag{11}$$

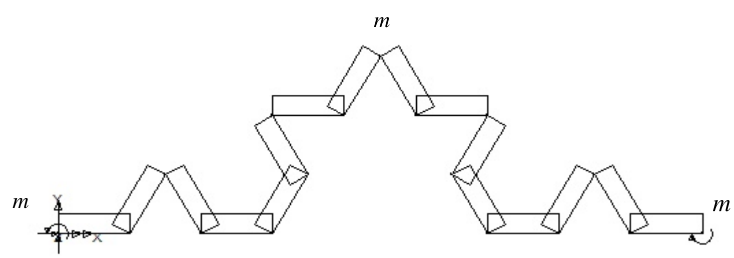

Figure 5. Diagram of the bending moment for a von Koch cantilever beam (step 2) subjected to a couple *m* at the free end.

On the other hand, if we suppose that the strain energy must be preserved, the rigidity k must increase and scale as:

$$k = EI \propto \left(\frac{4}{3}\right)^n . \tag{12}$$

Since the generation number n may be written in the form:

$$n = -\ln l_n / \ln 3 , \tag{13}$$

we have:

$$k = EI \propto l_n^{1-D} , \tag{14}$$

where D=ln 4\ln3 is the fractal dimension of the von Koch curve.
This is a simple, yet interesting, result: the rigidity k must increase if the strain energy Φ_n has to be conserved, due to the increased length L_n. Furthermore, it must scale exactly as l_n^{1-D} : in all the other cases, either the strain energy diverges or it converges to zero. The same occurs for the compliance.
If eqn.(14) keeps true, displacements at the free end clearly keep constant; for example, to what concerns rotation, we have (eqn.(9)):

$$\varphi_n = \varphi_0 , \quad \forall n . \tag{15}$$

3.3 VON KOCH CANTILEVER BEAM SUBJECTED TO A TRANSVERSAL FORCE AT THE FREE END

If the couple m is replaced by a transversal force F, the situation becomes a little more complex. In a generic section of the rectilinear cantilever beam the bending moment varies linearly:

$$M(x) = F(l - x), \tag{16}$$

whereas the shear force is constant and equal, in modulus, to F.
The related strain energy Φ_0 is:

$$\Phi_0 = \frac{1}{2}\int_S \frac{M^2}{EI}dx = \frac{1}{2}\int_0^l \frac{M^2}{EI}dx = \frac{F^2 l^3}{6EI}. \tag{17}$$

In this case, the Castigliano's Theorem provides immediately the value of the deflection v_0 at the free end:

$$v_0(x = l) = \frac{\partial \Phi_0}{\partial F} = \frac{Fl^3}{3EI}. \tag{18}$$

If a von Koch cantilever beam is now considered, it is necessary, for a structural analysis, to evaluate the strain energy related to the next iterations. An analytical expression is not so direct as in the previous case, since the bending moment M is not constant any more, but it varies linearly on each segment constituting the iterative structure (Figure 6).

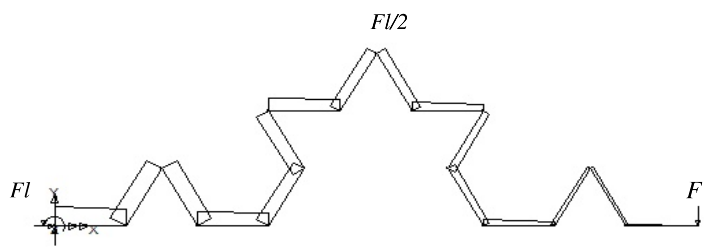

Figure 6. Diagram of the bending moment for a von Koch cantilever beam (step 2) subjected to a transversal force F at the free end.

In order to find a recursive relationship, we compute the strain energy for the first three iterations:

1. $\Phi_1 = \underbrace{\frac{34}{27}}_{B_1} \frac{F^2 l^3}{6EI} = \left(\frac{4}{3} - \frac{2}{27} B_0\right)\Phi_0$,

2. $\Phi_2 = \underbrace{\frac{1228}{729}}_{B_2} \frac{F^2 l^3}{6EI} = \left(\frac{16}{9} - \frac{2}{27} B_1\right)\Phi_0 = \left[\left(\frac{4}{3}\right)^2 - \frac{2}{27}\left(\frac{4}{3} - \frac{2}{27} B_0\right)\right]\Phi_0$

$\vdots$

n. $\Phi_n = \left[\left(\frac{4}{3}\right)^n - \frac{2}{27} B_{n-1}\right]\Phi_0 = \left[\left(\frac{4}{3}\right)^n - \frac{2}{27}\left[\left(\frac{4}{3}\right)^{n-1} - .... - \frac{2}{27} B_0\right]\right]\Phi_0$, (19)

where B_0=1 from eqn.(17). Thus, for n tending to infinity, the first term in the expression (19) dominates and all the other terms become negligible. The asymptotic result, for a sufficiently large n, is identical to that obtained in the previous case (i.e. applied couple): the strain energy Φ_n scales as the total length L_n. As a consequence, in order to preserve it, the rigidity k must scale as in eqn.(14). As n increases, the results converge, in this case, to those of the rectilinear cantilever beam (n=0):

$$\lim_{n\to\infty} v_n = v_0 \,. \tag{20}$$

3.4 NUMERICAL SIMULATIONS

In order to check the validity of the results obtained in the previous section, a FEA is performed by using the LUSAS ® code. Both the cases of the applied couple and force are considered.
The starting beam dimensions (i.e. the generator dimensions) are selected as follows: length l=1 m; area of the cross section A=0.4 10^{-3} m^2; moment of inertia I = 1.33 10^{-8} m^4. The material considered in the FEA is steel: the Young's modulus and Poisson's ratio are taken equal to E=2.09 10^{11} Pa and υ=0.3, respectively. A couple m equal to 100 Nm and a force F equal to 100 N are applied for the two contemplated cases.
Rotations and vertical displacements at the free end for the first four iterations of the von Koch cantilever beam are evaluated; according to eqn.(14), at each stage the beam rigidity k=EI is increased by a factor 4/3. The results are presented in Table 1.

Iteration	0	1	2	3	4	5
Rotation, $\varphi(m)$	0.03589	0.03589	0.03588	0.03586	0.03586	0.03586
Deflection, $v(F)$	0.01196	0.01130	0.01133	0.01135	0.01136	0.01137

Table 1. Rotation φ and deflection v [m] at the free end of a von Koch cantilever beam, due to a couple m=100 N m and to a force F=100 N, respectively.

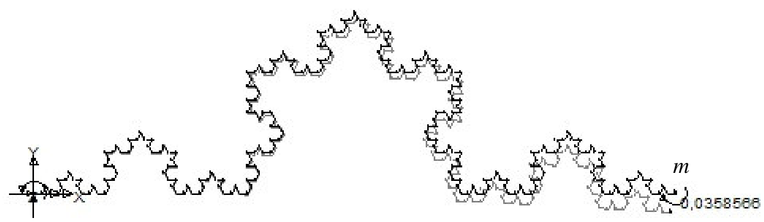

Figure 7. Elastic deformation and rotation at the free end of a von Koch cantilever beam (step 4) subjected to a couple m=100 N m.

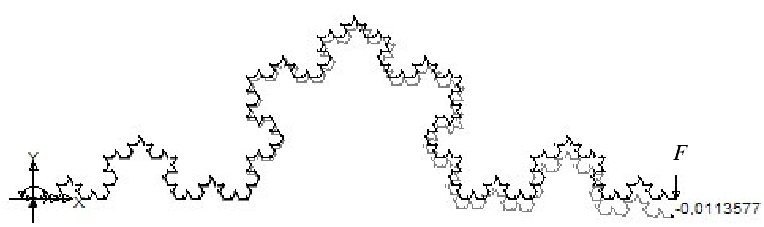

Figure 8. Elastic deformation and deflection [m] at the free end of a von Koch cantilever beam (step 4) subjected to a concentrated force F=100 N.

Therefore, as it can be seen, if the rigidity k scales as in eqn.(14), the results concerning the applied couple m are very close to those of a rectilinear cantilever beam, as deducible from eqn.(15) (Figure 7). On the other hand, displacements related to the force F converge, in the last case, to those of the generator as n increases, like expected from eqn.(20) (Figure 8).

4 CONCLUSIONS

In this paper a mathematical model to preliminary design nano-bio-inspired hierarchical materials, by following a bottom-up procedure, has been firstly proposed. The complexity of the problem has imposed a simplified treatment with associated limitations. The behaviour of hierarchical beam-framed structures, under different loading conditions, has also been analyzed. As an example of self-similar structure, the von Koch cantilever beam has been considered. Basic considerations on the strain energy conservation allow us to govern the structural response by scaling the geometric and mechanical features according to the length and the fractal dimension of the structure. Further studies are in progress.

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*Department of Structural Engineering and Geotechnics, Politecnico di Torino,
Corso Duca degli Abruzzi 24, 10129 Torino, Italy.*

*alberto.carpinteri@polito.it

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